Band structure fluctuation in pentacene thin film investigated by scanning probe microscopy

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In organic semiconductor devices, material inhomogeneity originating from defect, impurity, and grain boundary results in spatial fluctuation in the band structures. It has been well established that the spatial fluctuation dramatically impairs device performance of, for example, carrier mobility and threshold voltage. However, no direct observation of such fluctuation is reported. Here we report direct observation of the spatial distribution in the band structure using STM/STS and KFM.

A pentacene thin film was prepared by vacuum deposition at room temperature on an alkanethiol self-assembled monolayer (SAM) on a Au(111) substrate. Using STM, we confirmed that pentacene molecules are orderly packed with atomic steps (Fig. 1). For the STS measurement, I-V curves were measured at different areas, and the dI/dV-V curves were numerically calculated (Fig. 2). To obtain the spatial distribution of the band structure, the values of dI/dV for different V_s were imaged (Fig. 3).

The dI/dV-V curves reflect that a new state (gap state) is formed in the band gap of pentacene. The spatial distribution of the gap state has little relation with surface topography. We found that the gap state locates at the defect in the SAM. We propose that the gap state originates from the hybrid orbital between pentacene molecules and Au atoms.

Then we observed the surface potential for the same sample using KFM. We found that the surface potential has a similar spatial distribution to the gap state. This indicates that the charge transfer may be occurred via the gap state. Details will be discussed at the presentation.

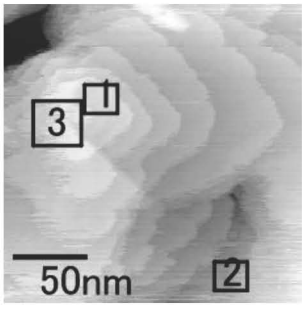

Fig. 1. STM topography of pentacene thin film.

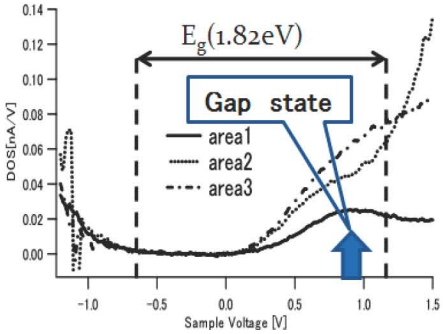

Fig. 2. dI/dV-V curves for different squared areas drawn in Fig. 1. Eg denotes bandgap of pentacene.

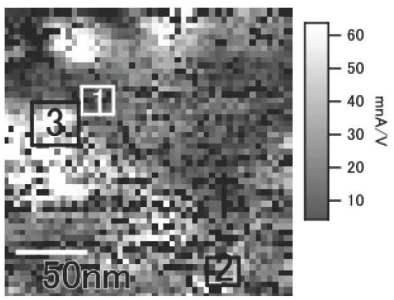

Fig. 3. dI/dV image for sample voltage of 0.8 V.